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This project has involved a quantitative theoretical interpretation of electron spectroscopic data with a view toward elucidating the chemical environment and electronic structure of atoms in the bulk and adsorbed on solid surfaces. Many-body effects, such as shake satellites, initial core hole screening, and final state hole-hole correlation, etc. have been examined and found to have significant effects on the spectral lineshapes. We have more recently examined electron spectroscopic data for the high temperature superconductors, and for chemisorbed species on metals. Electron/photon stimulated desorption (ESD/PSD) was also of interest. Here, an interpretation of spectroscopic data and comparison with PSD spectral yields was very helpful in obtaining an understanding of the image charge, surface resonances, polarization, and the role of many-body interactions in the desorption mechanism itself.

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QUANTITATIVE INTERPRETATION OF AUGER LINESHAPES AND ELECTRON/PHOTON STIMULATED DESORPTION

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d. Description of Project

This project has involved a quantitative theoretical interpretation of electron spectroscopic data with a view toward elucidating the chemical environment and electronic structure of atoms in the bulk and adsorbed on solid surfaces. Many-body effects, such as shake satellites, initial core hole screening, and final state hole-hole correlation, etc. have been examined and found to have significant effects on the spectral lineshapes. We have more recently examined electron spectroscopic data for the high temperature superconductors, and for chemisorbed species on metals. Electron/photon stimulated desorption (ESD/PSD) was also of interest. Here, an interpretation of spectroscopic data and comparison with PSD spectral yields was very helpful in obtaining an understanding of the image charge, surface resonances, polarization, and the role of many-body interactions in the desorption mechanism itself.

e. Significant Results

Table 1 summarizes our significant accomplishments in Auger spectroscopy, and Table 2 that in ESD/PSD. In each case, the tables indicate the system studied, the significance of the work, and the numerical sequence (as indicated below) of the papers (P) and technical reports (TR) published.

In summary we have shown that a very complex "many-body" experimental Auger spectroscopy can be used in a straightforward and simple manner to obtain important information on the electronic structure. On the other hand, we have shown that very complex "many-body" states are the primary actors in the ESD/PSD process, where previously very simple-minded one-body states were assumed to be the primary actor. By studying AES and ESD/PSD in the same context, we have shown that AES can be used to map the states responsible for the ESD/PSD process.

TABLE 1 - Review of Significant Accomplishments in AES

	SYSTEM	SIGNIFICANCE	PRODUCTIVITY (TR, P)*
1.	NO_3^-, SO_4^{2-} SiO_2	Proposed intermediate localization model. First det'm. of theo. shake/Auger lineshapes.	P- 1,2,6 TR- 1,4,7,14
2.	O_2 gas	First ab-initio determination of experimental Auger widths	P- 3,23 TR- 6,30
3.	NO_3^-	Effect of Mulliken vs. local populations on Auger intensity.	P- 4 TR- 5
4.	NO_3^-, O_2, C_2H_3, Cu, Be,	Proposed final state rule for Auger lineshapes.	P- 5,8,12 TR- 8
5.	C_6Li, C_8Cs	Proposed orthogonalized final state rule to account for enhanced intercalant peak	P- 7,9
6.	N_2, CO, O_2, NO	Systematic and consistent interpretation of spectra for diatomic molecules	P- 13,25,28,29 TR- 11,21,26,27,28
7.	Graphite	Established first case of localization in extended covalent system; first obs. of shakedown satellite.	P- 14,20,24,27 TR- 13,19,22,24
8.	Atoms with atomic # = 8-54	Det'm. of semi-empirical KVV and $L_{23}VV$ atomic Auger matrix elements.	P- 16
9.	TM carbides nitrides, oxides, SiC	Related Auger lineshapes to ionic bonding effects	P- 19 TR- 17
10.	Si	First quantitative interpretation of CCV Auger lineshapes;	P- 21 TR- 15
11.	Benzene Cyclohexane Polyethylene	Consistent interpretation and comparison of DU's in molecules and solids	P- 26,34,41 TR- 25,33,39,48
12.	Diamond	Established evidence for antiferromagnetic ordering on surface	P- 30 TR- 29

13.	Polyethylene, diamond	Established the role of excitation and shakeoff in AES processes.	P= 31 TR- 30
14.	Benzene, Transition metals	Interpretation of Auger line shapes for systems with less than 1/2 filled VB.	P- 32 TR -31
15.	Y-BA-Cu-O La-Sr-Cu-O	Interpretation of AES and XPS data indicates the Cu-O bond covalency correlates with T_c, and that no Cu^{3+} is present.	P- 37,43,44,45,46 TR- 37,43,44, 45,46,47
16.	C_2H_6/Ni, C_2H_4/Ni, CH/Ni	First quantitative interpretation of Auger line shapes for chemisorbed systems.	TR- 41

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*P and TR indicate sequence numbers of publications and ONR technical reports as listed below.

TABLE 2 **Summary of significant accomplishments in ESD/PSD.**

	SYSTEM	SIGNIFICANCE	PRODUCTIVITY (TR, P)*
1.	CO,N_2,H_2O	Established role of 2h1e type states in PSD of chemisorbed systems.	P- 10,11,15 TR- 9,10,12
2.	OH/Ti, Cr, Cu, O/Cr	Established the Auger induced desorption mechanism for non-maximal valency systems.	P- 19 TR- 18
3.	H_2O,OH/TiO_2 O/W,O/Mo	Resonant dissociative attachment mechanism found to be active for OH^* and O^-.	P- 22 TR- 23
4.	NH_3/Ru mixed N_2,O_2	Role of secondary electrons in desorption yields.	P- 18,38,40 TR- 16,36
5.	O_2/Ar/Pt	Elucidated the role of image charge effects in PSD.	P- 33,39 TR- 32
6.	O_2/Ar/Pt	Established the role of coherent scattering effects in the enhancement of ESD cross-section.	P- 35,42 TR- 34,40
7.	O_2/Pt,W	Elucidated the role of symmetry and its breakdown at surfaces in ESD	P-36 TR- 35,38,42

*P and TR indicate sequence numbers of publications and ONR technical reports as listed below.

f. Personnel who Worked on Project.

1. Dr. Hideo Sambe - Research Associate Professor
   Period worked: 11/1/81 - 3/15/89
   Understanding the nature of dissociation/desorption of small molecules and negative ion desorption.

2. Mr. Fred Hutson - Research Associate, part time
   Period worked 1/1/81 - 3/15/89
   Applications of electron spectroscopic data.

3. Mr. Hengxiang Yang - Graduate Student, partial summer support
   Period worked: 7/1/88-8/31/88
   Experimental study of thin films.

4. Dr. Wai-Ning Mei - Research Scientist
   Period worked: 5/19/81 - 3/31/82

5. Dr. Arnold Wahl - Research Professor
   Period worked: 11/01/81 - 12/31/81

g. Publications emanating from contract.

1. "Final State Correlation Effects in Auger Lineshapes, Application to Silicon Dioxide", D.E. Ramaker, Phys. Rev. **B21**, 6408 (1980).

2. "Auger Lineshapes of Solid Surfaces - Atomic, Bandlike, or Something Else?", B.I. Dunlap, F.L. Hutson, and D.E. Ramaker, J. Vac. Soc. Technol. **18**, 556 (1981).

3. "A Semiempirical X_a Calculation of the KVV Auger Line Shape of O_2", B.I. Dunlap, P.A. Mills, and D.E. Ramaker, J. Chem. Phys. **75**, 300 (1981).

4. "Interpretation of the N KVV Auger Lineshapes for Alkali Metal Nitrates", F.L. Hutson, D.E. Ramaker, B.I. Dunlap, J.D. Ganjei, and J.S. Murday, J. Chem. Phys. **76**, 2181 (1982).

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7. "Effect of Screening on the Carbon KVV Auger Lineshape of Alkali Intercalated Graphite", B.I. Dunlap, D.E. Ramaker, and J.S. Murday, Phys. Rev. **B25**, 6439 (1982).

8. "Initial and Final State Screening Effects in Auger Lineshapes", D.E. Ramaker, N.H. Turner, and W. N. Mei, J. Vac. Soc. Technol. **20**, 563 (1982).

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13. "Comparison of Autoionization and Photoemission Spectra for CO", M. Yousif, D.E. Ramaker, and H. Sambe, Chem. Phys. Letters. **101**, 472 (1983).

14. "Understanding Localized Behavior in the Auger Spectra of Covalent Systems such as Graphite", D.E. Ramaker, F.L. Hutson, R.R. Rye, J.B. Houston, and J.W. Rogers, J. Vac. Soc. Technol. **A2**, 1146 (1984).

15 "Photon-Stimulated Ion Desorption from Condensed N_2 and CO", H. Sambe, M. Yousif, and D.E. Ramaker, J. Vac. Soc. Technol. **A2**, 1011 (1984).

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25. "An Interpretation of the N_2 Photoelectron Spectrum", H. Sambe and D.E. Ramaker, Chem. Phys. Lett. **124**, 420 (1986).

26. "A Consistent Quantitative Interpretation of the Auger Lineshapes of Carbon in Molecules and Solids", D.E. Ramaker and F.L. Hutson, J. Vac. Sci. Technol. **A4**, 1600 (1986).

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33. "Image Charge Effects in Electron Stimulated Desorption: O^- from O_2 condensed on Ar Films Grown on Pt", H. Sambe, D.E. Ramaker, L. Parenteau and L. Sanche, Phys. Rev. Letters **59**, 236 (1987).

34. "Identification of Resonant Excitation and Shakeoff Contributions to the C KVV Auger Lineshapes of Several Gas Phase Hydrocarbons", F. Hutson and D.E. Ramaker, J. Chem. Phys. **87**, 6824 (1987).

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36. "The s- Selection Rule in Electron Attachment and Autoionization of Diatomic Molecules", H. Sambe and D.E. Ramaker, Chem. Phys. Letters **139**, 386 (1987).

37. "Observed Trends in the X-ray Photoelectron and Auger Spectra of High Temperature Superconductors", D.E. Ramaker, N.H. Turner, J.S. Murday, L.E. Toth, M. Osofsky, and F.L. Hutson, Phys. Rev. **B36**, 5672 (1987).

38. "Secondary Electron Effects in Photon Stimulated Desorption", D.E. Ramaker, T.E. Madey, R.L. Kurtz, and H. Sambe, Phys. Rev. B38, 2099 (1988).

39. "Image Charge, Coherent Scattering, and Symmetry Effects in Electron Stimulated Desorption: O^- from O_2 Condensed on Metals", D.E. Ramaker and H. Sambe, published in Desorption Induced by Electronic Transition, DIET III, ed by R. Stulen and M. Knotek, Springer Series in Surface Sci., (Springer, Berlin Heidelberg, 1988), p. 85.

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41. "Interpretation of the Ethylenic, Carbidic and Graphitic Auger Lineshapes of Chemisorbed Carbon Species", F.L. Hutson and D.E. Ramaker, J. Vac. Soc. Technol. **A6**, 1105 (1988).

42. "Electron Stimulated Desorption and Coherent Scattering", H. Sambe and D.E. Ramaker, J. Vac. Sci. Technol. **A6**, 836 (1988).

43. "Review of Photoelectron and Auger Data for the High Temperature Superconductors", D.E. Ramaker, In Thin Film Processing and Characterization of High Temperature Superconductors, J.M. Harper, J.H. Colton, L.C. Feldman eds, AVS Series No. 3, (AIP, New York, 1988) p. 284.

44. "Electron Spectroscopic Data for the High Temperature Suprconductors - What can We Learn from It?", D.E. Ramaker, Chemistry of High-Temperature Superconductors, edited by D.L. Nelson and T.F. George, ACS Symposium Series 377 (ACS, Washington, DC, 1988). p. 84.

45. "Utilization of a Hubbard U Model to Understand the Valence Band Photoelectron Data for the High Temperature Supercoductors", D. E. Ramaker, Phys. Rev. **B38**, 11816 (1988).

46. "Understanding Core Level Decay Processes in the High-Temperature Superconductors", D.E. Ramaker, N.H. Turner, and F.L. Hutson, Phys. Rev. **B38**, 11368 (1988).

h. Technical Reports Issued

1. "Final State Correlation Effects in Auger Lineshapes, Application to Silicon Dioxide", D.E. Ramaker.

2. "Symmetry of the Au(110) Surface Reconstruction Studied by Spin-polarized Low-Energy Electron Diffraction", B. Reihl and B.I. Dunlap.

3. "Symmetry Properites of Spin-polarized LEED", B.I. Dunlap.

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27. "Rydberg States Converging to the N_2^{++} Ionized States", H. Sambe and D.E. Ramaker.

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35. "The s^- Selection Rule in Electron Attachment and Autoionization of Diatomic Molecules", H. Sambe and D.E. Ramaker.

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40. "Electron Stimulated Desorption and Coherent Scattering", H. Sambe and D.E. Ramaker.

41. Interpretation of the Carbon Auger Line Shapes from Adsorbed and Fragmented Ethylene on Ni(100)", F.L. Hutson and D.E. Ramaker.

42. "Forbidden Electron Attachment in O_2", H. Sambe and D.E. Ramaker, submitted to Phys. Rev. B.

43. "Review of Photoelectron and Auger Data for the High Temperature Superconductors", D.E. Ramaker.

44. "Utilization of a Hubbard U Model to Understand the Valence Band Photoelectron Data for the High Temperature Supercoductors", D. E. Ramaker.

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46. "Electron Spectroscopic Data for the High Temperature Superconductors - What can We Learn from It?", D.E. Ramaker.

47. "Utilization of a Highly Correlated Cluster Model for Interpretation of Electronic Spectroscopic Data for the High Temperature Superconductors", D.E. Ramaker.

48. "Chemical Effects in the Carbon KVV Auger Line Shapes", D.E. Ramaker.

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